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**THE CALCULATION OF
THEORETICAL CHROMOSPHERIC MODELS AND
THE INTERPRETATION OF
SOLAR SPECTRA FROM ROCKETS AND SPACECRAFT**

NASA Grant NSG-7054

Final Report

For the period 1 July 1974 through 31 December 1992

**Principal Investigator
Eugene H. Avrett**

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**Smithsonian Institution
Astrophysical Observatory
Cambridge, Massachusetts 02138**

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1. INTRODUCTION

Since the early 1970s we have been developing the extensive computer programs needed to construct models of the solar atmosphere and to calculate detailed spectra for use in the interpretation of solar observations. This research involves two major related efforts: work by Avrett and Loeser on the Pandora computer program for non-LTE modeling of the solar atmosphere including a wide range of physical processes, and work by Kurucz on the detailed synthesis of the solar spectrum based on opacity data for over 58 million atomic and molecular lines. Our goals are 1) to determine models of the various features observed on the Sun (sunspots, different components of quiet and active regions, and flares) by means of physically realistic models, and 2) to calculate detailed spectra at all wavelengths that match observations of those features. These two goals are interrelated: discrepancies between calculated and observed spectra are used to determine improvements in the structure of the models, and in the detailed physical processes used in both the model calculations and the spectrum calculations. The atmospheric models obtained in this way provide not only the depth variation of various atmospheric parameters, but also a description of the internal physical processes that are responsible for non-radiative heating, and for solar activity in general.

A byproduct of our research will be the determination of the solar irradiance spectrum at all wavelengths versus solar activity as measured by various disk images. To the degree of accuracy that our calculated spectra agree with solar observations, we should be able to relate the intensity at one wavelength to that at any other wavelength in quiet or active regions anywhere on the solar disk. Thus we could compute needed solar irradiances at unobserved UV or EUV wavelengths based on available disk images in, say, the Ca II K line, the He 1083nm line, or from magnetograms, since irradiance variations are due almost entirely to the extent and location of active regions on the disk. Changes in the concentration of ozone and other molecules in the Earth's upper atmosphere are observed to be correlated with UV and EUV solar irradiance variations on time scales from a few days up to the 27-day period of solar rotation. Direct UV and EUV irradiance measurements during the last two 11-year solar activity cycles have been too few in number and too uncertain in absolute calibration to determine the solar input to long-term changes in the molecular chemistry high in the Earth's atmosphere. The calculated model spectra now may be accurate enough to reconstruct this past record of UV and EUV irradiance.

2. RECENT PROGRESS

Our collaboration with Edward Chang of the University of Massachusetts shows the interaction of these different aspects of our research. In 1983 Chang had identified the 12 μm solar emission lines as 6g-7h and 6h-7i transitions of Mg I, but no convincing explanation for the emission has been offered until recently. The lines were initially assumed to be chromospheric. Kurucz became aware of the JPL ATMOS experiment that flew on the space shuttle and took high-signal-to-noise infrared solar spectra that showed the bands of CO and hydrides in detail. These would be very useful for studying the temperature minimum region. Kurucz obtained the data, reduced them, determined the continuum level, and produced an atlas (that we will publish next year). Chang used this atlas to study the atomic emission lines at 7 and 12 μm and also to pick out all the Mg I lines. Then Chang and Avrett attempted to model the Mg I emission lines. They found that more and more sophisticated model atoms were required until a 41 level non-LTE calculation finally reproduced the behavior of the lines (Chang et al. 1991,1992). The model atom required many photoionization cross sections, collision cross sections, and transition probabilities. Chang and Kurucz were able to generate much of the required data. It turns out that the emission lines are formed in the upper photosphere and are in emission because the high-lying upper energy levels tend to be in equilibrium with the Mg II continuum while the lower-level populations are depleted due to radiative losses, causing the line source function to be larger than the Planck function for the 7 and 12 μm lines. The emission in these far infrared lines turns out to be sensitive to the effects of far-UV lines in the photoionization rates for the lowest levels of Mg I, which influence the corresponding radiative losses.

Avrett, Chang, and Loeser (1993) compare the ATMOS profiles of both Mg I and hydrogen lines in the 2.2 to 16.7 μm range with theoretical profiles calculated from atmospheric models corresponding to faint, average, and bright regions of the quiet sun. The Mg line profiles show only minor differences due to the models, while the H line profiles show large relative differences. The H lines can be used as diagnostics of atmospheric structure, while the Mg lines cannot. The Mg lines provide a strong test of various rates and cross-sections and of our non-LTE computational abilities.

We continued research on particle diffusion in collaboration with J.M. Fontenla of Marshall Space Flight Center. Fontenla, Avrett, and Loeser (1993) have shown that particle diffusion, in addition to thermal conduction, can bring down from the corona the energy needed to account for the observed emission from the lower transition region. As a result, the earlier semi-empirical transition region models have been replaced by theoretical energy-balance models. These theoretical models with steep gradients produce strong Lyman alpha emission because neutral hydrogen atoms diffuse upward to produce this emission near 40,000K rather than near the 20,000K temperatures in local statistical equilibrium calculations without diffusion. Protons diffusing downward from higher to lower temperatures carry ionization energy to supply the base of the transition region.

We are completing a detailed study of how the He I and He II lines are formed (Fontenla, Avrett, and Loeser, 1992; Avrett, Fontenla, and Loeser, 1993) and have not found any inconsistency between the computed and observed He I 58.4 and 1083 nm lines and 50.4 continuum and He II 30.4 and 164 nm lines and 22.7 continuum. Diffusion in the lower transition region may account for

the generally smaller and highly variable helium abundance in the solar wind, but that mass outflow and mixing in this region are needed to avoid a very small helium abundance in the corona. Diffusion may also explain the observed coronal abundance depletion of elements with high first ionization potential, since elements that are fully ionized in the low transition region would be subject to smaller differential effects of proton and neutral-atom diffusion.

On the basis of our experience with the ATMOS infrared spectra we feel that we have to pay much more attention to model atoms and to increasing the number of levels in non-LTE calculations. Chang will continue to work on improving model atoms for our non-LTE calculations and on detailed simulations of the lines of Mg, H, Na, Al, and Si. We will be able to use these to make improvements in the solar models themselves.

The Mg II h and k resonance lines are sensitive diagnostics of the upper chromosphere but the emergent line profiles can be strongly affected by the transition from complete redistribution in the core to coherent scattering in the wings. We are computing detailed h and k line profiles for our quiet sun and plage models including an improved treatment of partial frequency redistribution. This work is being carried out in collaboration with Han Uitenbroek who has developed a program to solve multi-level, non-LTE radiative transfer problems with a full treatment of partial frequency redistribution.

In collaboration with J.M. Fontenla we have taken the first steps to 1) include the diffusion of Mg atoms and ions in our models of the transition region and upper chromosphere, 2) study the effects of differential mass motions on the models, and 3) study the abundance variations induced by particle diffusion.

We attempt to compare our calculations with all available spectra. In some cases, this requires that we reduce or help to reduce the observed data to get them into usable form. Kurucz continued to work on the reduction of SMM, Kitt Peak FTS, and ATMOS spectra in the ultraviolet, visible, and infrared. We eventually plan to publish atlases with all the lines labelled. We also plan to produce an atlas of the solar spectrum with the effects of atmospheric absorption removed as much as possible from our ground based spectra.

Kurucz continued to add to and to correct his atomic and molecular line data. He is collaborating with Barbara Bell of Harvard College Observatory in iteratively computing the spectrum and comparing it to the observed spectrum to check for errors both in the line data and in the reduction of the observed spectrum.

Kurucz was able to compress all his line data into a few files that for the first time allow us to access all the line data on our VAXs instead of having to use a Cray. They are published on CDROMs. He wrote a new opacity sampling model atmosphere program that uses these compressed line files. Because the lines are treated explicitly it should be possible to modify the program to treat the lines in nonLTE or possibly to add the line subroutines to the Pandora computer program. Either approach will allow us to compute radiative rates much more accurately.

Figure 1 shows an LTE central intensity calculation with empirical Model C using all the lines from the list of 58 million for 200 to 300 nm. The upper line is the continuum level.

Figures 2 and 3 are sample calculations showing the difference between the spectrum computed with all the laboratory and predicted lines as above (thin line) and with just the laboratory lines (thick line) for 174 to 176 nm and for 160 to 162 nm. First, there are many more lines; much work remains to be done on atomic and molecular spectroscopy. Second the overall optical depth scale shifts upwards because the lines form an additional background opacity. The LTE emission is stronger because the height of formation is higher. It may not be possible to interpret individual features without treating all the lines that form a background.

Kurucz is completely revising his existing atomic molecular line lists using the new laboratory data that have become available over the last 10 years. He will add a number of minor species that were not needed in the earlier opacity calculations.

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